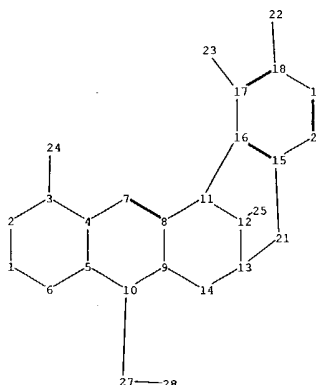


CAS Part 2 / 10
(Claim, 33, etc.)



FOR
CLAIM 33, etc.



chain nodes :
22 23 24 25 27 28 29 31 34
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21
ring/chain nodes :
30 32 33
chain bonds :
3-24 10-27 12-25 17-23 18-22 27-28 29-30 32-33 33-34
ring bonds :
1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-10 7-8 8-9 8-11 9-10 9-14 11-12 11-16 12-13
13-14 13-21 15-16 15-20 15-21 16-17 17-18 18-19 19-20
exact/norm bonds :
1-2 1-6 2-3 3-4 3-24 4-5 4-7 5-6 5-10 7-8 8-9 8-11 9-10 9-14 11-12 11-16
12-13 12-25 13-14 13-21 15-21 17-23 18-22 27-28 29-30 32-33 33-34
exact bonds :
10-27
normalized bonds :
15-16 15-20 16-17 17-18 18-19 19-20
isolated ring systems :
containing 1 :

1:H,CH3

2:H,OH,[*1],[*2],[*3]

match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom
22:CLASS 23:CLASS 24:CLASS 25:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:Atom
32:CLASS 33:CLASS 34:CLASS

generic attributes :

31:

Saturation

: Unsaturated

10/728580

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

ENTRY

TOTAL

SESSION

FULL ESTIMATED COST

155.84

156.05

FILE 'CAPLUS' ENTERED AT 19:03:05 ON 20 NOV 2004

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FILE COVERS 1907 - 20 Nov 2004 VOL 141 ISS 22

FILE LAST UPDATED: 18 Nov 2004 (20041118/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d his

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FILE 'REGISTRY' ENTERED AT 19:02:05 ON 20 NOV 2004

L1 STRUCTURE UPLOADED

L2 0 S L1

L3 4 S L1 SSS FULL

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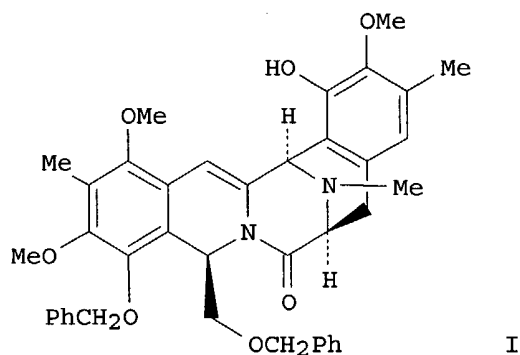
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L4 2 L3

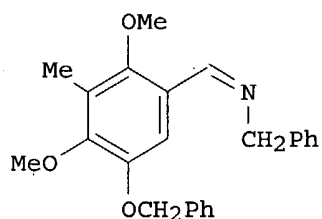
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10/728580

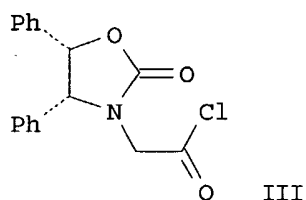
L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2003:382225 CAPLUS
DN 139:101312
TI Synthetic Studies on Ecteinasclidin-743: Constructing a Versatile
Pentacyclic Intermediate for the Synthesis of Ecteinasclidins and
Saframycins
AU Jin, Wei; Metobo, Sammy; Williams, Robert M.
CS Department of Chemistry, Colorado State University, Fort Collins, CO,
80523, USA
SO Organic Letters (2003), 5(12), 2095-2098
CODEN: ORLEF7; ISSN: 1523-7060
PB American Chemical Society
DT Journal
LA English
OS CASREACT 139:101312
GI



I



II



III

AB The asym. synthesis of a highly functionalized pentacyclic tetrahydroisoquinoline, I, relevant to the ecteinascidin, saframycin, safracin, and renieramycin family of antitumor alkaloids is described. I was prepared via Staudinger reaction of imine II with the ketene of acid chloride III and a Pictet-Spengler cyclization.

IT 557785-63-4P

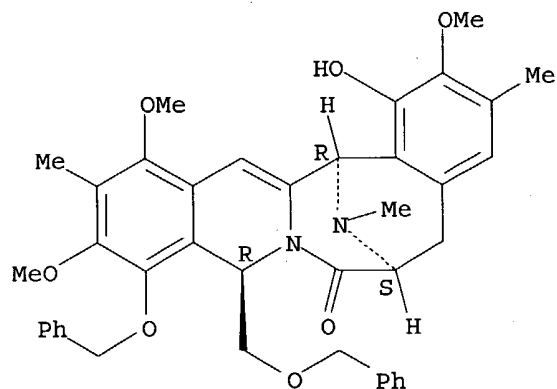
RL: SPN (Synthetic preparation); PREP (Preparation)
(asym. synthesis of pentacyclic isoquinoline as intermediate for ecteinascidins and saframycins via Staudinger and Pictet-Spengler reactions)

RN 557785-63-4 CAPLUS

CN 6,15-Imino-7H-isoquino[3,2-b][3]benzazocin-7-one, 5,6,9,15-tetrahydro-1-hydroxy-2,11,13-trimethoxy-3,12,16-trimethyl-10-(phenylmethoxy)-9-[(phenylmethoxy)methyl]-, (6S,9R,15R)-(9CI) (CA INDEX NAME)

10/728580

Absolute stereochemistry: Rotation (-).



RE.CNT 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/728580

L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN

AN 2001:545697 CAPLUS

DN 135:137633

TI Preparation of saframycin-ecteinascidin analogs and their therapeutic applications

IN Danishefsky, Samuel J.; Zhou, Bishan

PA The Trustees of Columbia University in the City of New York, USA

SO PCT Int. Appl., 115 pp.

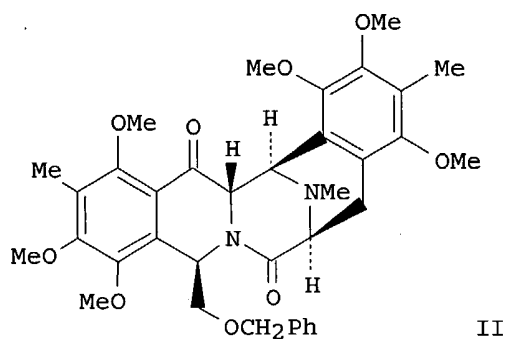
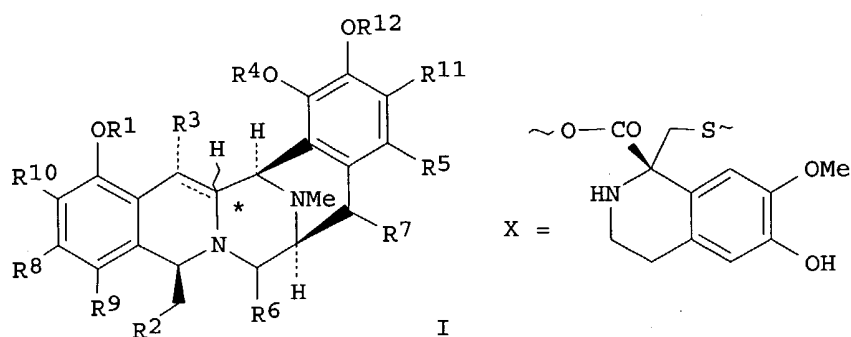
CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

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PI	WO 2001053299	A1	20010726	WO 2001-US1877	20010119
	WO 2001053299	C2	20021024		
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	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	CA 2397597	AA	20010726	CA 2001-2397597	20010119
	US 2002025962	A1	20020228	US 2001-765515	20010119
	US 6686470	B2	20040203		
	EP 1254140	A1	20021106	EP 2001-903151	20010119
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
	JP 2003520801	T2	20030708	JP 2001-553773	20010119
	US 2004127709	A1	20040701	US 2003-728580	20031205
PRAI	US 2000-177071P	P	20000119		
	US 2001-765515	A3	20010119		
	WO 2001-US1877	W	20010119		
OS	MARPAT 135:137633				
GI					



AB Compds. of the saframycin-ecteinascidin series such as I [R1,R4 = H, alkyl, acyl; R3 = =O, OH, ether, sulfide, acyl group such as OC(O)Me, OC(O)Bn and OC(O)Et; R5 = H, halogen, OH, ether, acyl, amide; R6 = =O, OH, OMe, CN, acyloxy; R7 = =O, OH, halogen, ether, acyl; R8 and R9 independently = H, Me, OMe, OEt, CF3, Br, F; R8R9 = OCH2O, five or six membered ring; R10,R11 = Me, OMe, OEt, SMe, SET; R12 = H, alkyl, acyl; chiral center marked * has the R or the S configuration], were prepared for use as antitumor and antimicrobial agents. Thus, saframycin analog II was prepared via a multistep synthetic sequence starting from 2,4-Dimethoxy-3-methylbenzaldehyde, bromoacetal, 2-hydroxy-4-methoxy-3-methylbenzaldehyde and [(2E)-4-bromo-2-butenyl]oxy(1,1-dimethylethyl)dimethylsilane. Ecteinascidin 743 I (R1 = Ac, R2R3 = X, R4 = R5 = R7 = H, R6 = α -OH, R8R9 = OCH2O, R10-R12 = Me) was tested for cytotoxicity and antimicrobial activity.

IT 351377-82-7P 351378-34-2P

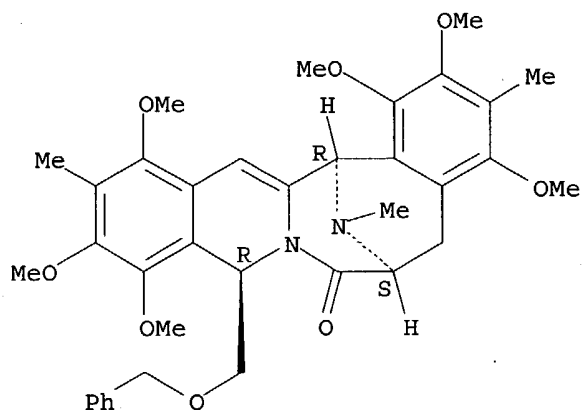
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of saframycin-ecteinascidin analogs and their therapeutic applications)

RN 351377-82-7 CAPLUS

CN 6,15-Imino-7H-isoquino[3,2-b][3]benzazocin-7-one, 5,6,9,15-tetrahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-9-[(phenylmethoxy)methyl]-, (6S,9R,15R)- (9CI) (CA INDEX NAME)

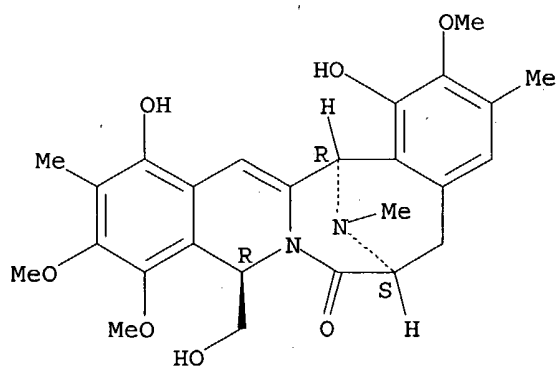
Absolute stereochemistry.



RN 351378-34-2 CAPLUS

CN 6,15-Imino-7H-isoquino[3,2-b][3]benzazocin-7-one, 5,6,9,15-tetrahydro-1,13-dihydroxy-9-(hydroxymethyl)-2,10,11-trimethoxy-3,12,16-trimethyl-, (6S,9R,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 351377-80-5P

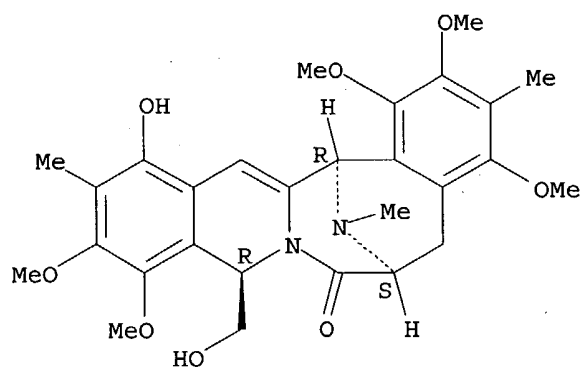
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of saframycin-ecteinascidin analogs and their therapeutic applications)

RN 351377-80-5 CAPLUS

CN 6,15-Imino-7H-isoquino[3,2-b][3]benzazocin-7-one, 5,6,9,15-tetrahydro-13-hydroxy-9-(hydroxymethyl)-1,2,4,10,11-pentamethoxy-3,12,16-trimethyl-, (6S,9R,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

10/728580



RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

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FILE COVERS 1907-1966

FILE LAST UPDATED: 01 May 1997 (19970501/UP)

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L5 0 L3

=> log h

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FULL ESTIMATED COST	0.42	166.87
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CA SUBSCRIBER PRICE	0.00	-1.40

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